

4-Aminoazobenzene
60-09-3 | DTXSID6024460

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 438 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.16e-01

Confidence level: 7.75e-01

Nearest Neighbors from the Training Set

Image not found

4-Aminoazobenzene

Measured: 617

Predicted: 438

Image not found

Chlorbufam

Measured: 162

Predicted: 235

Image not found

Phenylcarbamic acid butyl ester

Measured: 182

Predicted: 210

Image not found

N-Cyclopentyl-N'-phenylurea

Measured: 85.1

Predicted: 122

Image not found

Benzidine

Measured: 2880

Predicted: 1680